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THE USE OF DUAL RECIPROCITY BOUNDARY ELEMENTS FOR SIMULATION OF GROUNDWATER FLOW AND POLLUTANT TRANSPORT

T. I. Eldho and Der-Liang Young*
Department of Civil Engineering & Hydrotech Research Institute
National Taiwan University
Taipei, Taiwan 10617

B. Vasudeva Rao
Department of Civil Engineering
Indian Institute of Technology, Bombay
Mumbai, India 400 076

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ABSTRACT

The dual reciprocity boundary element method (DRBEM) has been established as an effective numerical tool in the modeling of various engineering problems. Here the application of the DRBEM in groundwater flow and pollutant transport is described. Several cases analyzed prove that DRBEM is an effective numerical tool in simulating these problems.

I. INTRODUCTION

Groundwater, in recent years, has been an important consideration in the water plans of many countries due to over exploitation and non-availability of surface water. In the development and management of groundwater resources, two major problems of interest are the quantity of available water and the quality of extracted water. For the efficient management of groundwater basins subjected to pumping and recharge, it is necessary to analyze and predict the hydraulic response of the system using effective tools. Similarly for the assessment of groundwater quality, it is necessary to identify the source of pollution and predict the movement of pollutants using effective techniques.

Generally, the hydrodynamic response of groundwater basins and pollutant movement in porous media are predicted using analytical, physical, field and numerical models. For the simulation of groundwater flow and pollution transport, very few exact analytical solutions are available and the physical and field models are cumbersome and difficult in practice. Hence, numerical models are in common use for the prediction of groundwater flow and pollution transport.

Commonly used numerical models are based on the finite difference method (FDM), the finite element method (FEM) and the boundary element method (BEM). FDM and FEM are in common use for the solution of groundwater flow and pollution dispersion problems for which domain discretization is required. For large-scale groundwater flow and pollutant transport problems, the discretization of the domain using FDM or FEM takes huge effort and the solution becomes cumbersome. Using BEM, if there

*Correspondence addressee

are no convective or time dependent terms in the governing equations, only the boundary of the domain is to be discretized for solution, hence, it is easier in field applications. But if there are convective terms or time dependent terms in the governing equations (which is the usual case with groundwater flow or pollutant transport problems), a solution using the general BEM (Brebbia, 1978) requires domain integration which reduces the attraction of the method.

The dual reciprocity boundary element method (DRBEM), converts all time dependent terms and convective terms into boundary integrals using a special technique and hence is totally boundary oriented. The internal points are defined wherever a solution is required. Hence, in DRBEM, a three dimensional problem is solved, computationally, in two dimensions and a two dimensional problem is solved, computationally, in one dimension. Here, the application of dual reciprocity boundary elements in the modeling of groundwater flow and pollution transport is briefly described, with some case studies.

The dual reciprocity boundary element method (DRBEM) was introduced by Nardini and Brebbia (1982) and was later generalized to a wide range of engineering problems (Partridge *et al.*, 1992). Various authors presented formulations for diffusion equations and diffusion-convection equations based on dual reciprocity boundary elements (De-Figueriredo and Wrobel, 1990; Partridge and Brebbia, 1992; Zhou and Zhang, 1994). Eldho (1995) used DRBEM for the solution of transient groundwater flow problems and pollution dispersion problems. Eldho and Rao (1997) presented the applications of DRBEM for two dimensional contaminant transport problems in porous media. In this paper, the general applications of DRBEM in groundwater flow and pollution dispersion modeling are described with the help of two case studies.

II. GROUNDWATER FLOW MODELING

1. Governing Equation and Formulation

The general governing equation for transient groundwater basin flow (both confined and unconfined aquifers) in homogeneous isotropic porous media can be expressed as Bear (1979):

$$\nabla^2\phi = \frac{1}{D}\frac{\partial\phi}{\partial t} - \frac{W}{T} \tag{1}$$

where ϕ- the potential or hydraulic head, T- the transmissivity of the aquifer, D- the diffusivity of the aquifer ($D=T/S$), S- storativity of the aquifer, t- the time and W- recharge or pumping rate (positive for recharge and negative for pumping). The following dimensionless form of variables are used in the solution:

$$X=x/L;\ Y=y/L;\ \Phi=\phi/\overline{\phi}\ ;\ t=\tau D_0/L^2;$$

$$\overline{W} = WL^2/T_0\overline{\phi}\ ;\ D'=D/D_0 \tag{2}$$

where L is a reference length, $\overline{\phi}$ is a reference hydraulic head, D_0 is a reference diffusivity, T_0 is the transmissivity corresponding to the reference diffusivity and τ is the time step.

For transient groundwater flow, the initial and boundary conditions should be prescribed. The initial condition, usually prescribed head, is described throughout the domain at some initial time. Two common types of boundary conditions may be defined in a typical aquifer problem. One is a Dirichlet condition (boundary of prescribed head) and another one is a Neumann condition (boundary of prescribed flux).

Considering the transient flow in aquifers without any pumping or recharge, Eq. (1) becomes,

$$\nabla^2\phi = \frac{1}{D}\frac{\partial\phi}{\partial t} \tag{3}$$

Here, in the solution of Eq. (3) using DRBEM, the time dependent term is approximated using the dual reciprocity method and then Green's theorem is applied to get a boundary solution. The fundamental solution of the Laplace equation is used for approximation. This procedure gives a boundary only solution with less complexity in the solution process of the governing equation.

In the dual reciprocity method, the term $\partial\phi/\partial t$ is approximated and Eq. (3) is represented as:

$$\nabla^2\phi = \frac{1}{D}\sum_{j=1}^{N+L} f_j(x,y)\alpha_j(t) = \frac{1}{D}\sum_{j=1}^{N+L} (\nabla^2\hat{\phi}_j)\alpha_j(t) \tag{4}$$

where f_j- a set of approximating functions, α_j- a set of initially unknown coefficients, N- number of boundary nodes, L- number of internal nodes and $\hat{\phi}_j$ is a series of particular solutions. Here the right hand side of Eq. (3) has been represented by a set of basis functions $f_j(x, y)$ multiplied by a set of unknown functions of time $\alpha_j(t)$ which in turn is replaced by a summation of products of coefficients α_j and the Laplacian operating on the particular solution $\hat{\phi}_j$. The number of $\hat{\phi}_j$ is equal to the number of nodes $N+L$.

Now, using the reciprocity principle on both sides of Eq. (4), discretizing the boundary into N linear elements and using L internal nodes, the boundary integral equation can be written in discretized form for a source node i as follows:

$$g_i\phi_i + \sum_{k=1}^{N}\int_{\Gamma_k}\frac{\partial\phi^*}{\partial n}\phi d\Gamma - \sum_{k=1}^{N}\int_{\Gamma_k}\phi^*\frac{\partial\phi}{\partial n}d\Gamma$$

$$= \frac{1}{D}\sum_{j=1}^{N+L}\alpha_j(g_i\hat{\phi}_{ij} + \sum_{k=1}^{N}\int_{\Gamma_k}\frac{\partial\phi^*}{\partial n}\hat{\phi}_j d\Gamma - \sum_{k=1}^{N}\int_{\Gamma_k}\phi^*\frac{\partial\hat{\phi}_j}{\partial n}d\Gamma) \quad (5)$$

where ϕ^* is the fundamental solution of the Laplace equation, n is the unit outward normal and g_i is Green's constant; g_i=1 for a point inside the domain, g_i=0 for a point outside the domain and $g_i=\theta/2\pi$ for a point on the boundary, in which θ is the internal angle at point i in radians.

After introducing the interpolation function and integrating over each boundary element, applying to all boundary nodes using a collocation technique and using the initial and boundary conditions, a system of linear equations can be formed. The solution of this linear system of equations gives the unknown function values first on the boundary of the domain and then the internal values can be found from Eq. (5). The detailed formulation of DRBEM for groundwater flow can be found elsewhere (Eldho, 1995, 1996).

The approximating function 'f' used here is '$1+r$' where r is the distance from the point i of application of the concentrated source or sink to any other point under consideration. Here the pumping and recharge effects (Eq. 1) are considered as concentrated sinks and sources (Brebbia, 1978).

The presented model has been compared with one analytical solution given in Liggett and Liu (1983) and one FEM model given in Pinder and Gray (1977) for confined aquifer conditions (Eldho, 1995). Here the comparison with the analytical solution is presented. The aquifer considered is a square region of unit dimension without any pumping or recharge and unit diffusivity. On the left hand side of the domain boundary, unit potential ($\phi(0, y, t)$=1.0) and right hand side of the domain boundary zero potential ($\phi(1, y, t)$=0.0) are assumed. On other boundaries, no flow boundary condition ($\partial\phi/\partial n$=0) are assumed. Initially, throughout the domain zero potential ($\phi(x, y, 0)$=0.0) are assumed. Here, dimensionless variables as given in Eq. (2) are used. For the problem described, the exact analytical solution is described in Ligget and Liu (1983).

In the DRBEM model, the boundary of the domain is discretized into 20 linear elements and 12 internal nodes are considered and a dimension-less time step of 0.05 is used. Figure 1 shows the potential variation with respect to time at various points in comparison with the analytical solution. Good agreement is observed between the DRBEM solution and the analytical solution. In the transient groundwater flow analysis using DRBEM, the accuracy and stability of the results depend on the use of optimal dual reciprocity boundary element model parameters like time steps, number of boundary elements, number of internal nodes, weighting factors and approximating functions used in the investigation. A detailed sensitivity study of these parameters can be found in Eldho (1996).

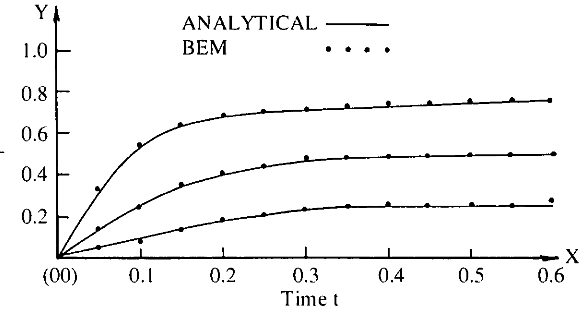

Fig. 1. Comparison of ϕ variation for DRBEM model and analytical solution

2. Case Study

To show the effectiveness of DRBEM in groundwater flow analysis, a case study of regional aquifer modeling is presented here. An unconfined aquifer in Pochampad Ayacut, Andhra Pradesh, India is considered to determine the effects of continued pumping on the regional groundwater basin (Eldho, 1995). The aquifer considered has a specific area of 67 sq.km. It is wedge shaped bounded by two streams, Peddavagu and Kortalavagu, on two sides and the Pochampad main canal on the third side as in Fig. 2. Groundwater mainly occurs in this basin under unconfined conditions. From the pumping tests, the average transmissivity and storativity are observed to be 79.5 m^2/day and 4.55×10^{-3} respectively. For the study purpose, the aquifer is considered to be homogeneous and isotropic. The two boundary streams are considered as recharging boundaries. The other boundary, the Pochampad main canal is a lined canal, having been excavated beyond the average depth of weathering in the region, and is assumed to be impermeable. The groundwater levels available in 1971 without any pumping effect varying from 270 to 304 m, are taken as the initial groundwater levels for the purpose of analysis. All these data are taken from the publication of Baig and Prabhakar (1980).

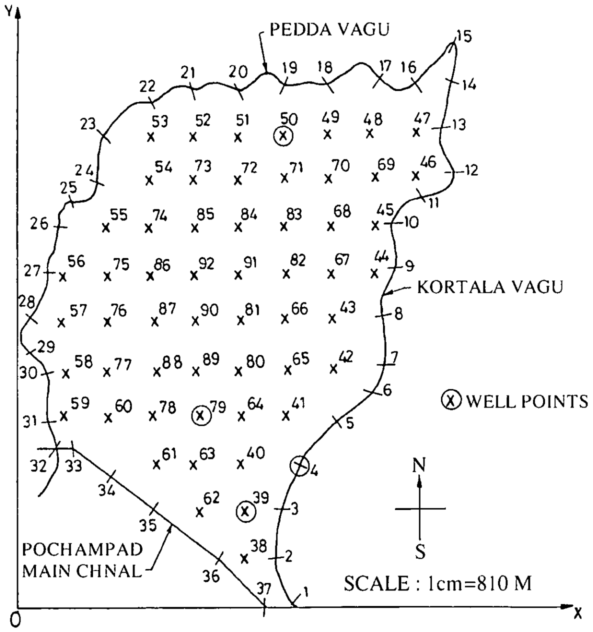

Fig. 2. Aquifer plan and DRBEM discretization

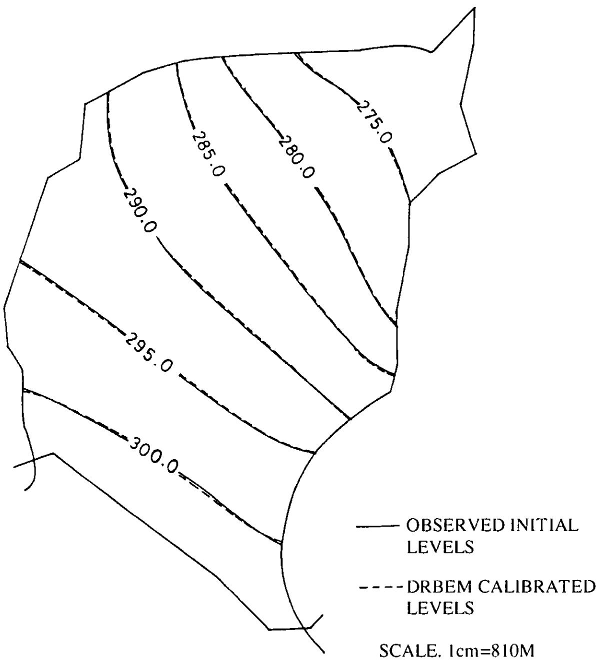

Fig. 3. Model Calibration - case study

3. Calibration of The Model

For the simulation of a real aquifer, it is essential that the model used is calibrated with the initial data available so that the model reflects back the response of the original situation within reasonable limits. In the present case study, the data available is a record of initial water levels observed in 1971, when there was no pumping. No data is available about the recharging stream boundaries. Hence, in the absence of any other data, the initial water levels of 1971 have been considered as the unknown steady state solution of potential head distribution over the entire basin. A steady state analysis is carried out for calibration. The boundary of the domain is discretized into 37 linear elements and 55 internal points are considered as in Fig. 2. From the given conditions and initial boundary heads, the fluxes (discharges and recharges) at the boundary nodes and the heads at internal points are predicted. These boundary recharges and discharges are assumed to exist over future times as the boundary conditions of the basin in addition to the future prescribed pumping activities.

To ascertain the accuracy of the calibrated model, the boundary discharges and recharges are redistributed to see whether given boundary heads and internal nodes are obtained, if so, the model is calibrated. The calibrated groundwater levels and the initially observed water levels of 1971 are plotted in the form of contours in Fig. 3. Both the contours agree closely and establishes the validity of the calibration.

4. Prediction of Future Transient Water Levels with Pumping

For the prediction of future transient water levels with pumping effects, a case study is considered with pumping wells located at nodal points 4, 39, 50 and 79 (see Fig. 2) pumping at a rate of 169, 169, 338 and 338 m^3/day respectively. The pumping wells are treated as concentrated sinks in the model (Brebbia, 1978). The boundary of the domain is discretized into 37 linear elements and 55 internal points are considered to find the potential distribution. The recharge and discharge rates obtained from steady state analysis are used as boundary conditions. The given initial potential is described as the initial condition on the nodes and a time step of 1 day is used in the analysis. The groundwater levels are predicted at the end of 1 year, 5 years and 10 years, due to continuous pumping and the corresponding contours are shown in Fig. 4. The potential variation at some selected nodes (42, 53, 63, 70, 77 and 92) with respect to time is shown in Fig. 5.

This case study shows the effectiveness of DRBEM in groundwater flow modeling. The transient groundwater flow problem with pumping and recharge is solved entirely based on boundary discretization. Internal points are defined wherever a solution is needed. Using DRBEM, the two dimensional problem is solved computationally in one dimension. The irregular shape of the boundaries of the problem is considered such that computation is not possible with other numerical methods, only with

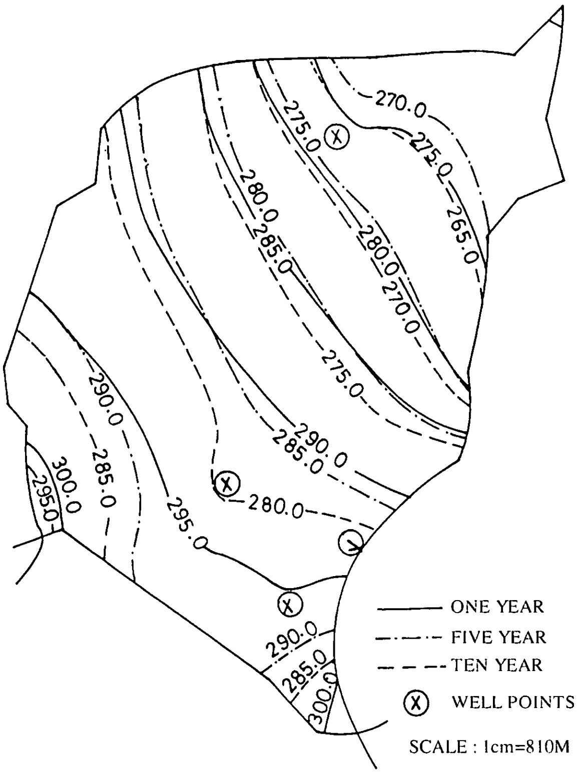

Fig. 4. Contours of predicted potential - case study

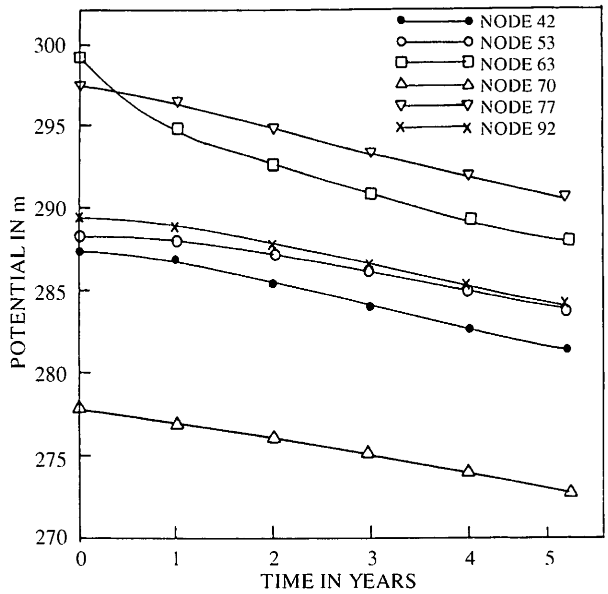

Fig. 5. Potential variation with time - case study

DRBEM. The pumping and recharge are considered as concentrated sinks and sources. As is clear from the case study, the data required and prepared are much less than needed by other numerical methods.

III. GROUNDWATER POLLUTANT TRANSPORT MODELING

1. Governing equation and formulation

The two-dimensional governing equation for groundwater contaminant transport in saturated, homogeneous and isotropic porous media (Van Genuchen *et al.*, 1977) can be expressed as:

$$D_{xx}\frac{\partial^2 C}{\partial x^2} + D_{yy}\frac{\partial^2 C}{\partial y^2} = R\frac{\partial C}{\partial t} + \frac{1}{n_e}(U_x\frac{\partial C}{\partial x} + U_y\frac{\partial C}{\partial y}) + \lambda RC \tag{6}$$

where C is the pollutant solution concentration, D_{xx} and D_{yy} are the dispersion coefficients in x and y directions, t is the time, U_x and U_y are the Darcy velocity components in x and y directions, n_e is the effective porosity, R is the retardation factor of the porous media and λ is a first-order decay constant for solutes that undergo decay. A dimensionless form of Eq. (6) can be achieved by substituting,

$$c = \frac{Cn_e}{C_0}\ ;\ X = \frac{x}{L'}\ ;\ Y = \frac{\beta y}{L'}\ ;\ u_x = \frac{U_x L'}{D_{xx}}\ ;$$

$$u_y = \frac{\beta U_y L'}{D_{xx}}\ ;\ t' = \frac{D_{xx}t}{L'^2} \tag{7}$$

in which C_o and L' are some reference concentration and length and $\beta=(D_{xx}/D_{yy})^{1/2}$.

To solve a particular problem, the governing equation has to be supplemented by appropriate initial and boundary conditions. The initial condition, usually prescribed concentration, is described throughout the domain at some initial time. Two boundary conditions are commonly used in the solution of pollution dispersion problems. One is a Dirichlet condition (boundary of prescribed concentration) and another one is a Neumann condition (boundary of normal gradient of the concentration).

Here in the solution of the dispersion equation using DRBEM, the time dependent term and convective terms are approximated using the dual reciprocity method and then Green's theorem is applied to get a boundary solution. The fundamental solution of the Laplace equation is used for approximation. This procedure gives a boundary only solution with less complexity in the solution process and allows any of the coefficients to have variable values without adopting special techniques. Assuming D_T as the longitudinal dispersion coefficient, $V_x=U_x/n_e$, $V_y=U_y/n_e$ and using Eq. (7) (while keeping the symbols same as in Eq. (6)), then

$$\nabla^2 C = \frac{1}{D_T}(V_x\frac{\partial C}{\partial x} + V_y\frac{\partial C}{\partial y} + \lambda RC + R\frac{\partial C}{\partial t}) = \frac{b}{D_T} \tag{8}$$

In the DRBEM, the right hand side of Eq.(8) can be represented as:

$$\nabla^2 C = \frac{1}{D_T}\sum_{j=1}^{N+L}\alpha_j(\nabla^2\hat{C}_j) = \frac{1}{D_T}\sum_{j=1}^{N+L} f_j(x,y)\alpha_j(t) \qquad (9)$$

where $\hat{C}_j$ is a series of particular solutions, N is the number of boundary nodes, L is the number of internal nodes, α_j is a set of initially unknown coefficients and f_j are approximating functions. Here, the right hand side of Eq. (9) has been represented by a set of coordinate functions $f_j(x, y)$ multiplied by an unknown function of time $\alpha_j(t)$, which in turn is replaced by a summation product of coefficients α_j and the Laplacian operating on the particular solution $\hat{C}_j$. The number of $\hat{C}_j$ is equal to the total number of nodes $N+L$.

Now using reciprocity principle on both sides of Eq. (9), discretizing the boundary into N linear elements and using L internal nodes, the boundary integral equation can be written in discretized form for a source node i as follows:

$$g_i C_i + \sum_{k=1}^{N}\int_{\Gamma_k}\frac{\partial C^*}{\partial n}C d\Gamma - \sum_{k=1}^{N}\int_{\Gamma_k} C^*\frac{\partial C}{\partial n}d\Gamma$$

$$= \frac{1}{D_T}\sum_{j=1}^{N+L}\alpha_j[g_i\hat{C}_{ij} + \sum_{k=1}^{N}\int_{\Gamma_k}\frac{\partial C^*}{\partial n}\hat{C}_j d\Gamma$$

$$-\sum_{k=1}^{N}\int_{\Gamma_k} C^*\frac{\partial \hat{C}_j}{\partial n}d\Gamma] \qquad (10)$$

where C^* is the fundamental solution of the Laplace equation, n is the unit outward normal and g_i is Green's constant, as defined earlier.

After introducing the interpolation function and integrating over each boundary element, applying to all boundary nodes using a collocation technique and using the initial and boundary conditions, a system of linear equations can be formed. The solution of this linear system of equation gives the unknown function values first on the boundary of the domain and then the internal concentration values can be found from Eq. (10). The detailed formulation of DRBEM for pollution dispersion in porous media can be found elsewhere (Eldho and Rao, 1997).

The approximating function 'f' used here is '$1+r$' where r is the distance from the point i of application of the concentrated source or sink to any other point under consideration.

The DRBEM model has been compared with some one-dimensional and two-dimensional analytical solutions (Eldho and Rao, 1997). Here, the comparison with one analytical solution is presented. The porous media considered is a rectangular region of 600m×100m size and is homogeneous, isotropic and fully saturated. The longitudinal dispersion coefficient of the media (D_T) is assumed to be 7.616 m^2/day, the retardation factor R=1.0, radioactive decay coefficient is assumed to be zero, seepage velocity = 1.219 m/day and source fluid discharge is assumed to be zero. On the left hand side of the domain boundary, unit relative concentration ($C(0, y, t)$ =1.0) and on the right hand side of the domain boundary zero relative concentration ($C(600, y, t)$=0.0) is assumed. On other boundaries, no flow condition and derivative of concentration ($\partial C/\partial n$=0) is assumed as zero. Initially, throughout the domain zero concentration ($C(x, y, 0)$=0.0) is assumed. Here, dimensionless variables, as given in Eq. (7), are used. For the problem described, the exact analytical solution is described in Marino (1974).

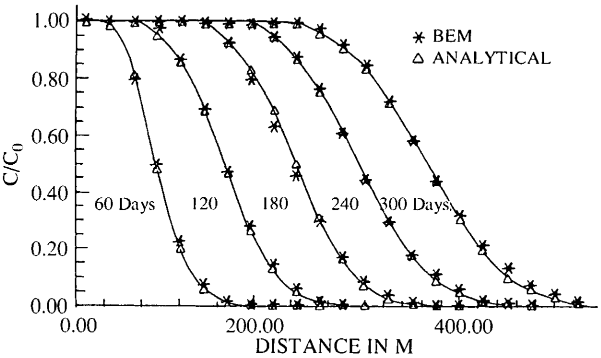

Fig. 6. Comparison of pollutant distribution for DRBEM and analytical solution

In the DRBEM model, the boundary of the domain is discretized into 52 linear elements and 11 internal nodes are considered and a time step of 1 day is used. The dispersion analysis is carried out for 300 time steps and concentration distribution is found. Figure 6 shows the relative concentration distributions along the domain at various times in comparison with the analytical solution. Good agreement is observed between the DRBEM solution and the analytical solution.

As in the case of groundwater flow modeling, the accuracy, stability, convergence and computational efficiency of the DRBEM model for pollutant dispersion analysis also depends on the use of optimal dual reciprocity boundary element model parameters like time steps, boundary discretizations, internal nodal distributions, weighting factors and approximating functions used in the investigation. A detailed sensitivity study of these parameters can be found in Eldho and Rao (1997).

IV. CASE STUDY

To show the effectiveness of DRBEM in

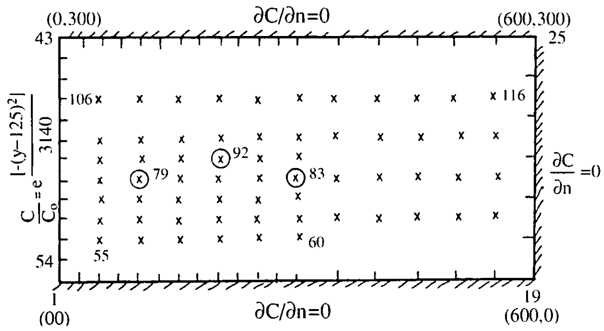

Fig. 7. Solution region for pollution dispersion case study with discretization

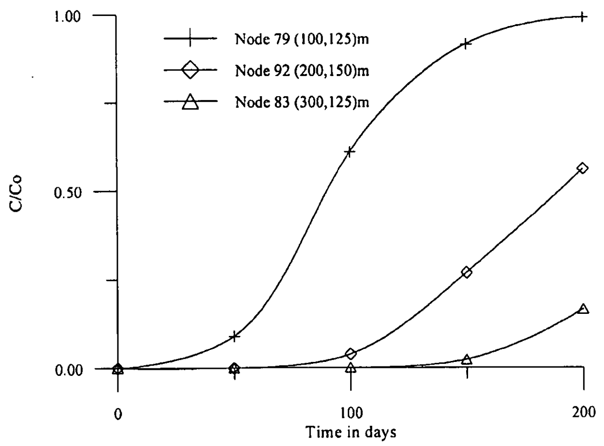

Fig. 8. Solute concentration distribution with time

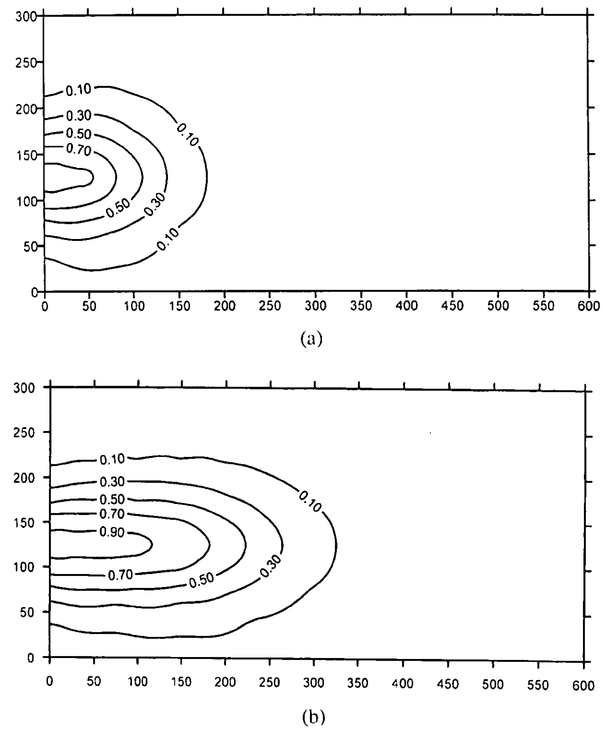

Fig. 9. (a) Contours of the relative pollutant distribution after 100 days. (b) Contours of the relative pollutant distribution after 200 days

groundwater pollution analysis, a case study of pollution dispersion in an aquifer is presented here. An unconfined aquifer of domain size 600m×300m is considered to determine the effects of pollution dispersion in porous media (Eldho, 1995). The boundary of the domain is discretized with 54 linear elements and 62 internal nodes are used. Fig. 7 shows the discretization with the input concentration that varies along the y-axis. The dispersion coefficient in the x- direction (D_{xx}) is 7.622 m^2/day and in the y-direction (D_{yy}) is 0.4795 m^2/day. The unidirectional seepage velocity through the aquifer media is 1.22 m/day.

A time step of 2 days is used in the analysis. The pollutant dispersion analysis is carried out for 200 days. Figure 8 shows the concentration development with time at three nodes, 79 (100, 125), 92 (200, 150) and 83 (300, 125). Figs. 9a and 9b show the contours of the relative pollutant concentration distribution after 100 days and 200 days from the beginning of the pollution. To analyze the pollution movement after stopping the contamination source, numerical analysis is continued for 200 more days after the removal of the contamination source. Figs. 10a and 10b show the relative contours of the pollutant concentration distribution 100 days and 200 days after stopping the contamination source (300 days and 400 days after the beginning of the pollution).

This case study shows the effectiveness of DRBEM in groundwater pollutant transport modeling. The time dependent and convective terms in the governing equation are approximated in such a way that the problem is solved entirely based on boundary discretization. Internal points are defined wherever a solution is needed. Using DRBEM, the two dimensional, problem is solved computationally, in one dimension. In the present model, the effect of numerical dispersion is found to be negligible compared to other numerical methods (Eldho and Rao, 1997). As is clear from the case study, the data required and prepared are much less than compared to other numerical methods.

V. CONCLUDING REMARKS

Here the applications of the dual reciprocity boundary element method in the analysis of groundwater flow and pollution modeling are described. The time-dependent term and convective terms in the diffusion equation and dispersion equation are approximated using the dual reciprocity method to achieve a boundary only solution. Various case

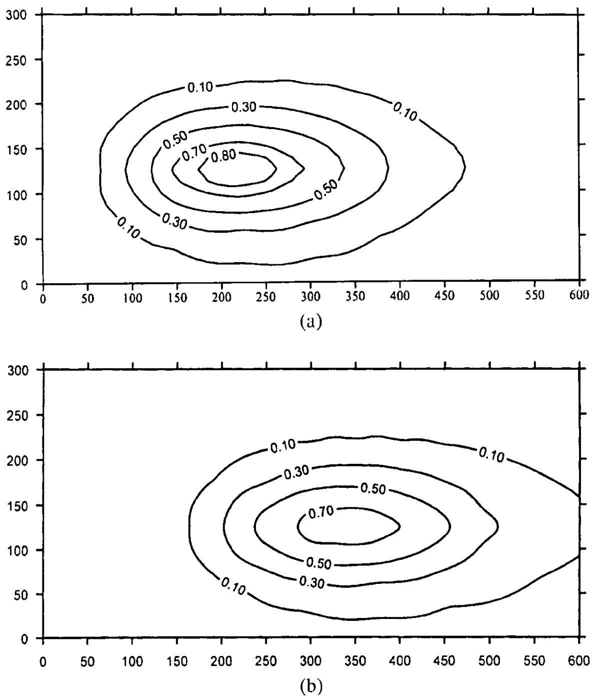

Fig. 10. (a) Contours of pollutant distribution after the source removal (100days). (b) Contours of pollutant distribution after the source removal (200days)

studies analyzed show the effectiveness of the DRBEM in groundwater flow and pollution dispersion analysis. In DRBEM, all the basic advantages of the BEM, like reduction in computational dimension, ease of data handling and less numerical dispersion are achieved. DRBEM is particularly advantageous in the analysis of large groundwater basins with irregular boundaries as only the boundary of the domain is discretized and internal nodes are considered at the desired points.

NOMENCLATURE

C	pollutant solution concentration
C^*	fundamental solution of Laplace equation
D	diffusivity of the aquifer
D_{xx}, D_{yy}	Dispersion coefficient in x, y directions
f_j	approximating functions
g_i	Green's constant
L	number of internal nodes
N	number of boundary nodes
n	unit outward normal
n_e	effective porosity
R	retardation factor
S	storativity of the aquifer
t	time
T	transmissivity of the aquifer
U	Darcy velocity
W	recharge or pumping rate

Greek symbol

ϕ	potential
λ	first order decay constant
τ	time step
α	a set of initially unknown coefficients
ϕ^*	fundamental solution of Laplace equation

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以雙倒易邊界元素法模擬地下水流及污染物傳輸

T. I. Eldho 楊德良

國立台灣大學士木工程學系暨水工試驗所

B. V. Rao

印度孟買印度理工學院土木工程學系

摘 要

雙倒易邊界元素法已廣泛有效地被利用於模擬各種工程上的問題，本文利用雙倒易邊界元素法應用於地下水流及污染物傳輸之研究，許多例子証明雙倒易邊界元素法對於處理這種問題是一十分有效率的數値工具。

關鍵詞：地下水，污染物擴散，雙倒易邊界元素法。